

REBUS-3/DIF3D Code Upgrades for Support of VHTR Analysis

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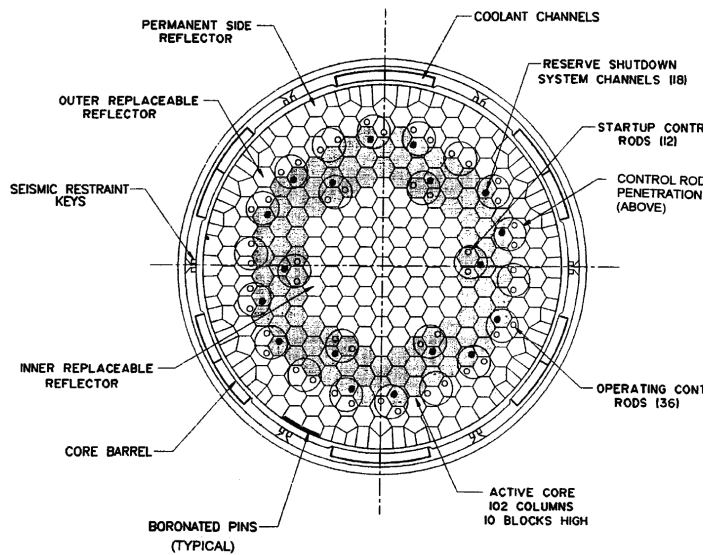
Overview

- **Background**
- **Objective**
- **Assessment and Selection of Initial Suite of Codes**
- **FY 2006 Planned Activities**
- **Accomplishments**
- **Conclusions**

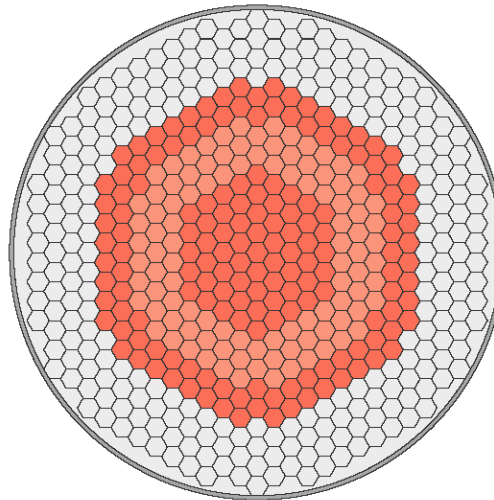
Background

- **Very high temperature reactor (VHTR) is a leading candidate for the next generation nuclear plant (NGNP)**
- **Physics analysis of VHTR requires modeling capabilities**
 - Double heterogeneity of coated particle fuel
 - Neutron streaming in coolant channels
 - Power peaking at core and reflector interface
- **Monte Carlo codes have these capabilities, but they are still too expensive to use in extensive design calculations**
 - Several important phenomena are not properly addressed yet (e.g. thermal feedback)
- **Deterministic code systems used for design and analysis of HTGRs are generally based on old technology in pedigree and platform**
 - Approximate methods and cumbersome to use
- **It is desirable to adapt modern deterministic tools for VHTR analysis and to verify and validate them**

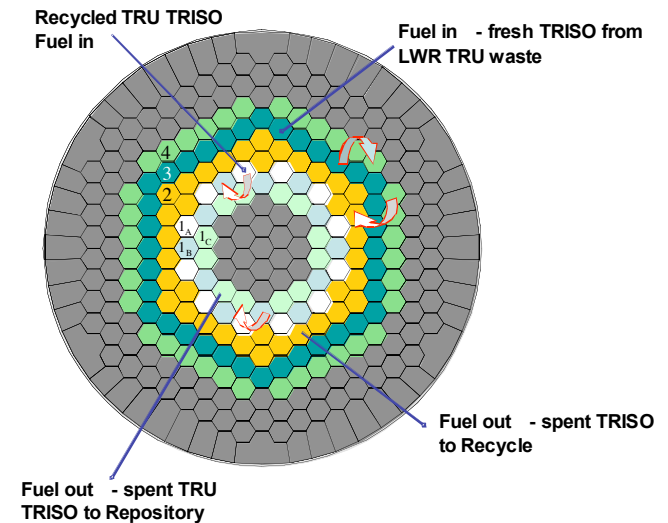
Experiences of Whole Core Depletion Calculations using DIF3D/REBUS-3 Code System



VHTR



LS-VHTR



DB-MHR

- Whole-Core Depletion Studies in Support of Fuel Specification for Next Generation Nuclear Plant Core
- Preliminary Neutronics Studies for the Liquid-Salt-Cooled Very High Temperature Reactor
- Feasibility Study of Deep Burn Concept

Objective

- **Develop a suite of advanced deterministic codes that can be used for efficient and accurate analysis of VHTR designs**
 - Develop deterministic two-step procedure for whole-core analysis
 - Evaluate accuracy of code package
 - Incorporate advanced models in code suite
 - *E.g., Adapt DeCART code for analysis of VHTR designs (originally developed for PWR analysis in previous I-NERI project)*

Assessment of Deterministic Whole-Core Analysis Tools

- **Deterministic whole-core analysis tools were evaluated**
 - Literature survey and assessment
 - Preliminary evaluation of DIF3D/REBUS-3 code system of ANL (without thermal feedbacks)
- **There are a number well-established deterministic tools expected to be applicable to VHTR analyses**
 - Modifications are required to address unique modeling issues of VHTR
 - Their performances for VHTR applications need to be verified and validated
- **Available capabilities need to be integrated into a code suite for VHTR analysis**
 - Assembly lattice codes, whole-core static and depletion analysis capabilities, and spatial kinetics tools, etc
- **Integrated code suite needs to be verified and validated**

Selection of Initial Suite of Codes

Lattice codes

- **DRAGON and WIMS9 were selected because of their capability to treat double heterogeneity of particulate fuel and availability**

Whole-core analysis codes

- **DIF3D/REBUS-3 system was selected since it can be adapted to prismatic VHTR analysis with limited effort compared to other codes**
 - Capable of multi-group flux and microscopic depletion calculations
 - Various geometry models including hexagonal-Z geometry
 - Nodal diffusion and transport theory capabilities
 - Equilibrium and non-equilibrium fuel cycle analysis capabilities
 - External cycle modeling

Two-Step Procedure

■ DRAGON & WIMS9

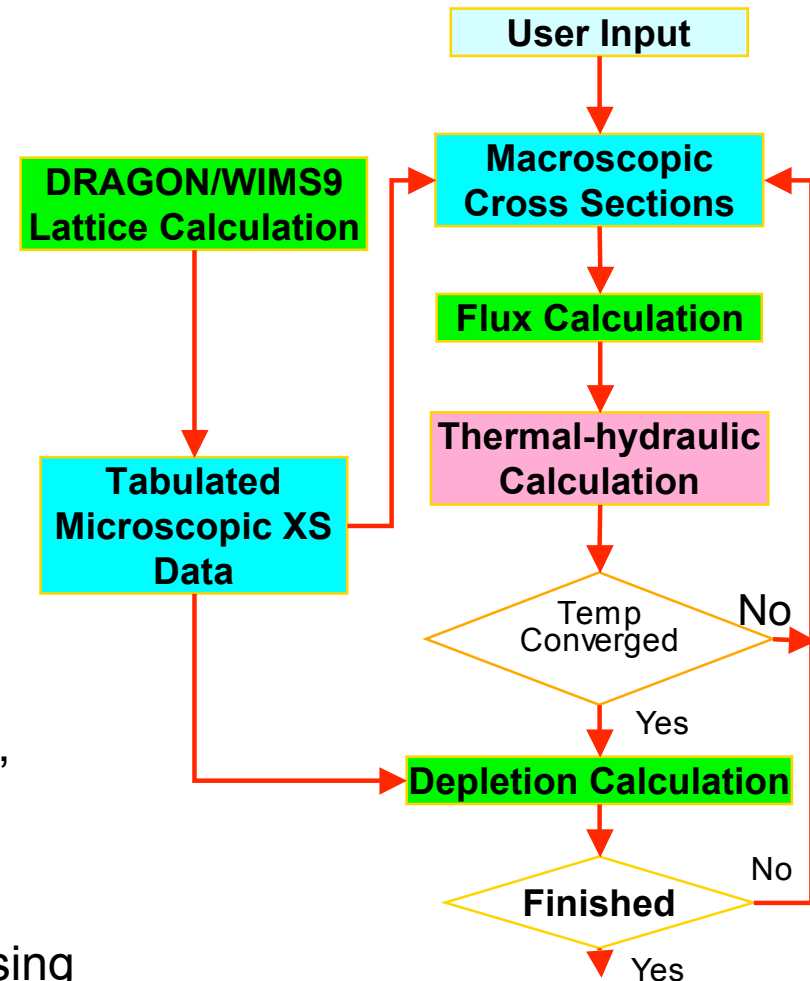
- Double heterogeneity treatment

■ DIF3D/REBUS-3

- Multi-group diffusion & transport
- Various geometry models
- Equilibrium fuel cycle analysis
- External cycle modeling

■ Cross Section functionalization

- Tabulation scheme (burnup, fuel temperature, moderator temperature, packing fraction, ...)
- Multi-dimensional table lookup
- Random access file for rapid processing



Required Developments and Enhancements

■ **Processing code for generating functionalized cross-section library**

- Evaluation of cross section dependencies on state variables
- Development of cross-section functionalization scheme
- Development of processing code

■ **DRAGON and WIMS9**

- Improved resonance treatment

■ **DIF3D/REBUS-3**

- Implementation of functionalized cross section library and interpolation scheme
- Implementation of thermal-hydraulic computational module and thermal feedback scheme
- Extension of nodal capabilities to incorporate use of nodal equivalence parameters and directional diffusion coefficients

FY 2006 Planned Activities

- **Enhance REBUS-3/DIF3D model for neutronic analysis of prismatic block VHTR**
 - Implement algorithms for T-H feedback and pin/compact power reconstruction
 - Improve algorithms for nuclide evolution
- **Develop a cross-section functionalization scheme linking DRAGON or WIMS9 assembly calculations to DIF3D/REBUS-3 whole-core analysis**
 - Evaluate the dependencies of VHTR (block-type) fuel element cross sections on various state variables using results of the DRAGON or WIMS8 lattice codes
 - Develop a cross section functionalization scheme and a code for “automated” processing of homogenized multigroup cross sections for the fuel and reflector and control blocks
 - *Nodal equivalence theory parameters and directional diffusion coefficients will also be considered to account for the homogenization errors expected in the regions where significant material discontinuities exist - e.g. at the core/reflector interface and control rod regions*
 - Implement a functionalized cross-section library and interpolation scheme in REBUS-3/DIF3D for VHTR (block-type) analysis

Accomplishments: Development of Cross-Section Functionalization Scheme

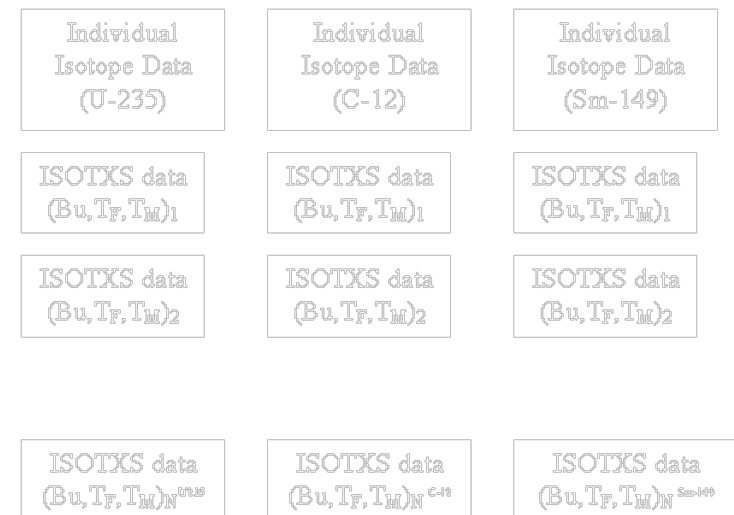
- **A new cross section storage procedure, called NEUTRONXS, was developed**
 - Fortran 90 object orientated data structures facilitate depletion calculations using user-defined depletion chain and based on microscopic cross sections of each isotope (large memory requirement)
- **A scattering cross section management module, COMPACTSCAT, was written with the working object being a single block of banded scattering data**
 - This approach to the storage reduces the memory usage and is straightforward to transfer to and from disk
- **Module GENERALISOTOPE was developed with the working object being a complete set of individual isotopic microscopic cross section data (total, transport, capture, fission, nu, etc.)**
 - Scattering data was included as a component data type
 - Optional polynomial dependencies for all of the microscopic cross section data also included
- **A utility program was written that takes the isotopic cross section data from DRAGON and WIMS9 lattice calculations for individual assemblies and merges them into a single NEUTRONXS file**

NEUTRONXS

■ A Multi-variable User-definable Tabulation Scheme

- Accumulates microscopic cross section data from WIMS and/or DRAGON lattice calculations
- General multi-variable tabulated data format was defined using isotopic based data structure
- Each table point contains microscopic (ISOTXS) cross section data with specific variable properties (burnup, temperature, etc...)
- All data is stored in random access file for rapid processing. Table interpolation is recursive requiring semi-layered table layout.
- Lumped fission product treatments along with homogenized compositions are supported (isotopes which have weak variable dependencies)

Table Header
Energy Group Details
Isotope Names
Property Data for each stored set of
ISOTXS data

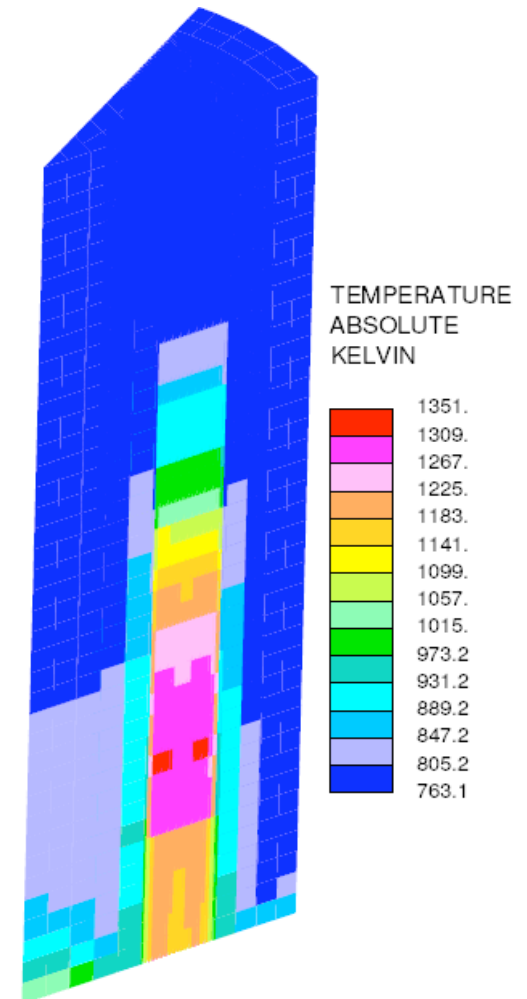
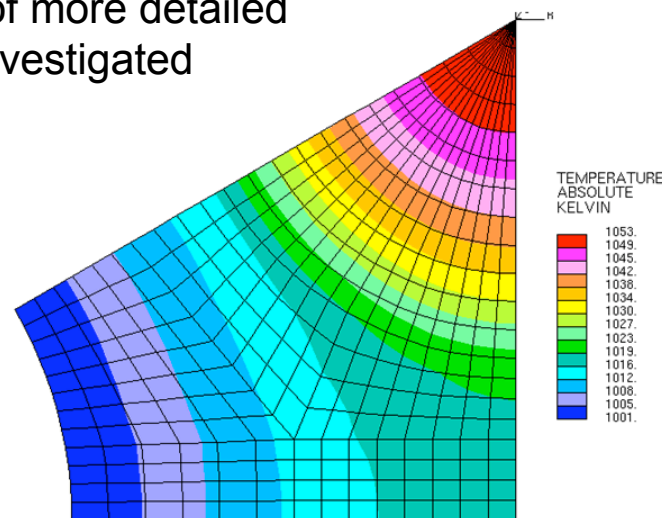


Accomplishments: Enhancement of REBUS-3/DIF3D Model

- **REBUS-3 modules and DIF3D driver routines reformatted and recompiled in Fortran 90**
 - Verification benchmark calculations successfully executed
- **Capability to treat variable burnup time steps implemented in REBUS-3 in order to model properly the initial fission products buildup**
- **A new Fortran 90 routine, DIFFERENTIALBURNUP was prepared to obtain material and stage dependent burnups for use in the calculation of burnup dependent cross sections**

Thermal-Hydraulics Model

- **As a first step to implement thermal feedback for static and depletion analyses, a simple unit cell heat conduction model was developed**
 - Axial variation of heat transfer coefficient is small ($< \sim 5\%$)
 - Axial heat conduction can be neglected (axial temperature gradient $< \sim 1.5\%$ of radial gradient)
 - Effective 1-D heat conduction model is reasonable for calculating radial heat conduction in unit cell
 - Implementation of more detailed model is being investigated



Verification of the Depletion Capability

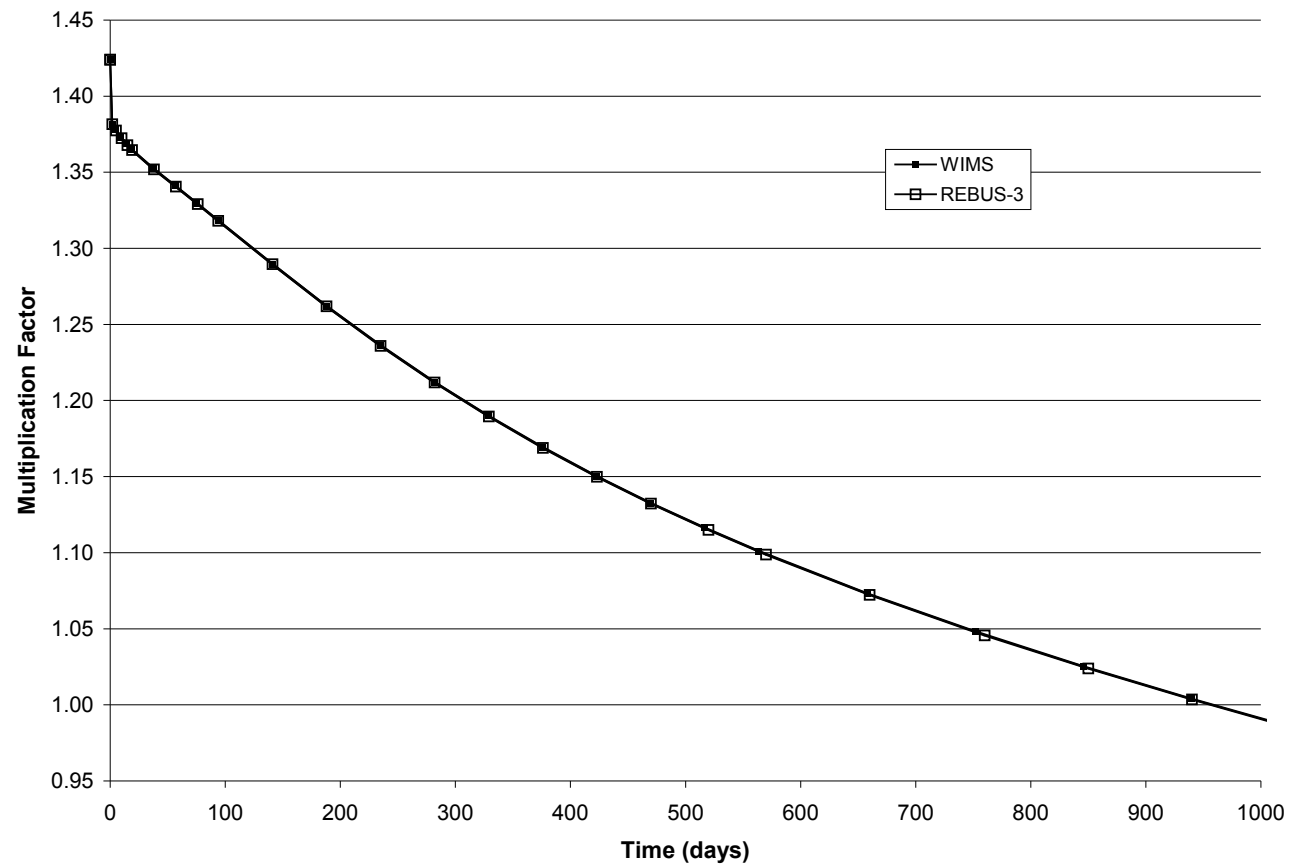
■ **Single Assembly Calculations**

- With lumped fission product treatment
- Without lumped fission product treatment
- Reference solution obtained with WIMS or DRAGON code
- Results should be “identical”

■ **Simple Core Problem**

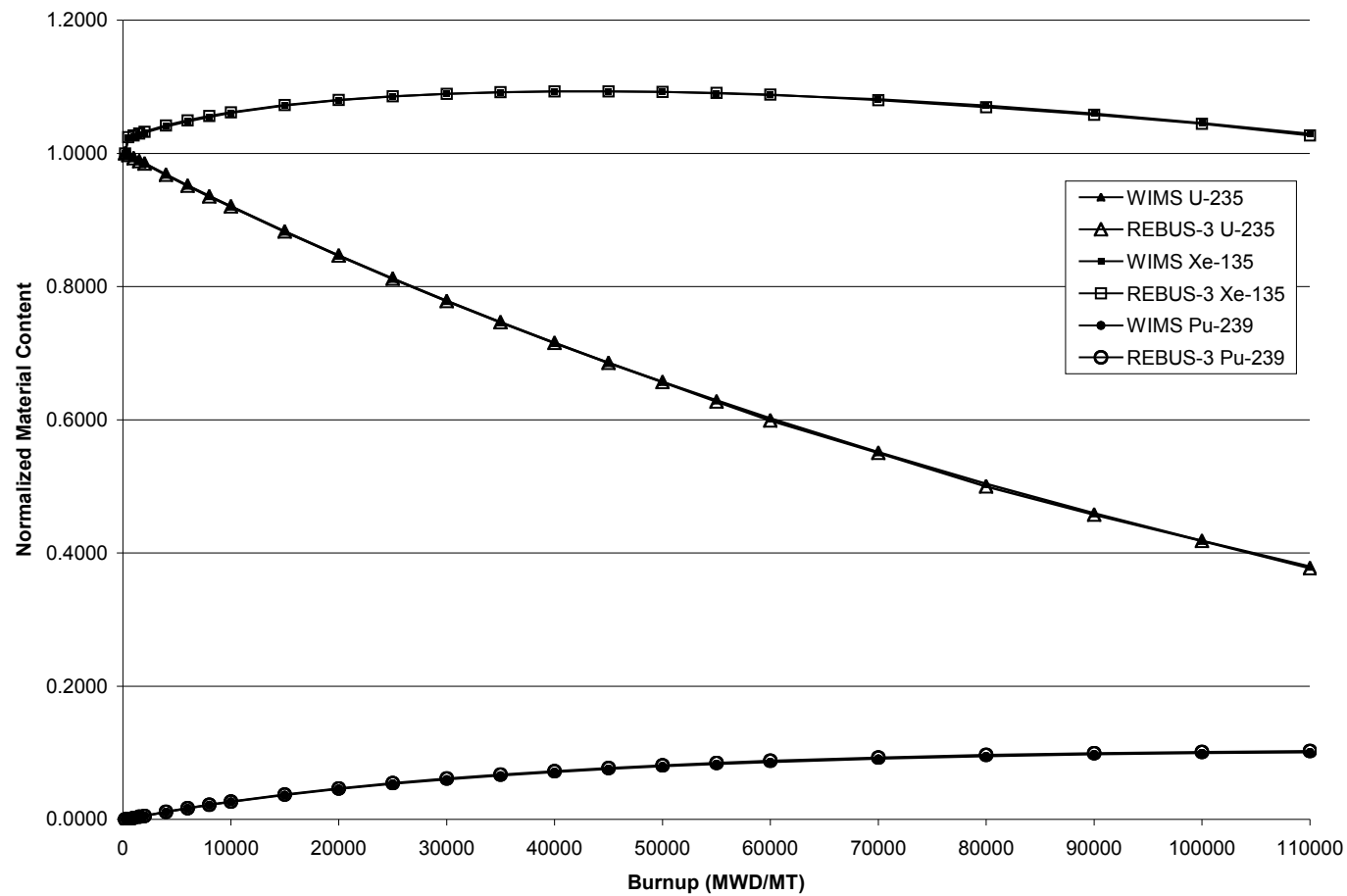
- Loaded entirely with fresh fuel
- Effectively a R-Z problem so radial rings were merged in depletion calculation (quick turnaround)
- No reference result

Uranium Assembly with WIMS Data



- Explicit modeling of ~80 fission products, 6 energy groups

Material Destruction



Conclusions

- **Lattice and whole-core capabilities for VHTR analyses were assessed**
- **Initial suite of codes for VHTR analysis was selected and required enhancements were identified**
 - Lattice codes: DRAGON and WIMS8
 - Whole-core calculation tools: DIF3D/REBUS-3
- **Required development and improvements are being implemented**
 - Cross section processing and fitting codes are being developed for interfacing assembly lattice and whole-core calculations
 - Modifications to REBUS-3/DIF3D ongoing

Backup

- Backup
- Backup
- Backup

DIF3D Code

- DIF3D is multigroup diffusion and transport theory solver
- Problem Types
 - Eigenvalue problem
 - Adjoint flux problem
 - Fixed source problem
 - Criticality (concentration) search
 - Nodal transport kinetics capability (coupled to SAS4A)
- Flux solution options
 - Finite difference diffusion theory method (DIF3D)
 - *Cartesian, cylindrical, spherical, and triangular geometries*
 - Nodal diffusion theory method (DIF3D-Nodal)
 - *Cartesian and hexagonal geometries*
 - Variational nodal transport theory method (VARIANT)
 - *Cartesian and hexagonal geometries*

VARIANT

- Motivated by need to improve the transverse-integration nodal method in hexagonal-z geometry
- VARIANT (**V**ariational **a**nisotropic **n**odal **t**ransport)
 - Solves multi-group transport problems in 2D and 3D Cartesian and hexagonal geometries with anisotropic scattering
 - Combines spherical harmonics or simplified spherical harmonic expansion in angle with hybrid finite element treatments of the spatial variables
 - *Angular spherical harmonic or simplified spherical harmonic approximations (maximum P_{99} or SP_{99})*
 - *Orthogonal polynomials for spatial approximation (maximum 99th order flux, 9th order leakage)*
- Additional capabilities
 - Pin flux and power reconstruction
 - Adjoint and perturbation capabilities
 - Nodal transport kinetics capability (coupled to SAS4A)
 - Sub-element capability for heterogeneous nodes

Capabilities of REBUS-3

- REBUS-3 was designed for fast reactor fuel cycle analysis
 - Equilibrium cycle analysis
 - *Equilibrium conditions of a reactor operating under a periodically repeating fuel management*
 - Non-equilibrium cycle analysis
 - *Explicit cycle-by-cycle operation of a reactor under a specified periodic or non-periodic fuel management program*
- Flexible user-defined burnup chains
 - No limit on number of nuclides
 - Ten reaction types
 - (n, γ) , (n, f) , (n, p) , (n, α) , $(n, 2n)$, (n, d) , (n, t) , β^- , β^+ , α
- Various neutronics flux solvers available
 - All the noted DIF3D options, TWODANT, and MCNP
- External cycle model
- Diverse search options including fuel enrichment, discharge burnup, control poison density, and burn cycle time

REBUS-3: External Cycle Modeling

- Position-dependent discharged atom densities
- Flexible reprocessing
 - User-specified allocation of discharge fuels to multiple reprocessing plants
 - Isotope-dependent recovery factors
- Flexible re-fabrication
 - Multiple reprocessing plant outputs and external feeds
 - User-specified multi-level priority scheme for distributing available atoms to different fuel types
- Modeling for time delays between various processes and radioactive decays

REBUS-3: Equilibrium Cycle Analysis

- Equilibrium cycle results typically used for design calculations
 - Limiting cycle achieved after an infinite number of burn cycles for a fixed fuel management scheme
 - Provides generic estimates of burn cycle time, control requirements, fuel enrichments
 - Results are valid for “average” core performance
- Cyclic-mode equilibrium cycle is a two-point boundary value problem
 - Fresh fuel composition depends on discharge fuel compositions and external cycle models
- Additional constraints
 - Charged fuel enrichment to satisfy the un-poisoned multiplication factor at a specified time
 - Cycle length to satisfy the constraint on the maximum discharge burnup
 - The control poison density can be adjusted to maintain the system criticality at each time node